40 Years of Diffraction Line Profile Analysis: from Scherrer Equation to Whole Powder Pattern Methods

P. Scardi[1]

[1]*Department of Civil, Environmental & Mechanical Engineering, University of Trento, via Mesiano 77, 38123 Trento, Italy*

Email: Paolo.Scardi@unitn.it

Diffraction techniques have the main purpose of providing structural information on the atomic-scale organization of matter, primarily crystalline materials. However, the diffraction pattern also contains information on the microstructure, in terms of shape, size and dispersion of the crystalline domains and the disorder present, both chemical and structural in nature. Most of this microstructural information is contained in the profile of the diffraction peaks, with additional characteristics related to the diffuse scattering component.

The study of peak profiles started in 1918, a few years after the discovery of X-ray diffraction, with the work of Paul Scherrer, a student of Peter Debye in Göttingen. Different and more complete methodologies have been proposed in the following years, but the strong diffusion of Line Profile Analysis (LPA) mainly concerns the last 40 years, with the advent of computers and specific software for the study of powder diffraction patterns. This has led to further methodological developments, and above all a growing integration between structural and microstructural analyses.

In particular, convolutional methods are now available to describe and analyse the diffraction pattern collected over an extended angular range, to obtain information based on physical models of the studied materials. The evolution of these methods over the last 25 years is briefly proposed here, with my personal contributions and application examples based on analysis with specific software for Whole Powder Pattern Modelling (WPPM), but also commercially available software, e.g., Topas, equipped with appropriate macros for WPPM. In addition to the LPA, I'll consider the diffuse scattering component, often overlooked and confused with the background in common powder pattern analyses, but actually rich in information on disorder of both a static and dynamic nature. The proposed approach, which takes care of both the description of the diffraction profiles and the diffuse component, presents itself in all respects as a total scattering method. With this approach, in addition to the microstructural information provided by WPPM, it is possible to obtain details on the correlation of thermal and static atomic displacements. The comparison of the results of this approach with more traditional methods based on the Pair Distribution Function (PDF) is also shown, with case studies based both on atomistic modelling with Molecular Dynamics and with real case studies concerning nanocrystalline and strongly deformed materials.

The list of everyone I would like to thank would perhaps be too long for this abstract, so I sincerely thank everyone, and in particular my many students and coworkers, who over the years have provided me with collaboration and concrete contributions, as well as constant motivation to develop a deeper understanding of powder diffraction. Teaching what I have learned has been a formidable tool for both professional and human growth.
Nothing I have done would have ever been possible without the fundamental support of my family, my wife Emilia, my children and their partners, and in recent years of my beloved granddaughter Matilde.